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New York, NY 10003 -

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14. ABSTRACT

We proposed to address the scientific and engineering challenges associated with developing and demonstrating DNA-based wave-guiding devices that incorporate radiation-sensitive bio-molecules to define new architectures that can be used to control and manipulate information propagation at the nanoscale. Prof. N. Seeman, of New York University (NYU), has led the effort to define an advanced methodology for the precision-placement of self-assembled bio-systems and implement structures that incorporate frequency-selective, radiation-sensitive

15. SUBJECT TERMS

Controlled DNA Structures; Designed Materials; 2D; 3D; Self-Assembly, Photonic Band Gap Materials

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Nadrian Seeman
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Report Title

Final Report -- DNA-Based Photonic Bandgap Structures and Devices

ABSTRACT

We proposed to address the scientific and engineering challenges associated with developing and demonstrating DNA-based wave-guiding devices that incorporate radiation-sensitive bio-molecules to define new architectures that can be used to control and manipulate information propagation at the nanoscale. Prof. N. Seeman, of New York University (NYU), has led the effort to define an advanced methodology for the precision-placement of self-assembled bio-systems and implement structures that incorporate frequency-selective, radiation-sensitive molecular elements. Prof. Seeman remains the world-leader in DNA-based nanofabrication and has pioneered methods (e.g., Seeman tiles) for the construction of periodic/aperiodic and symmetric/asymmetric bio-structures. Prof. H.-L. Cui, of Stevens Institute of Technology (SIT) has led the effort for defining the DNA-based photonic bandgap crystal devices and perform physics-based modeling of their wave-guiding properties. Prof. Cui is an expert in solid-state physics and electronics, and has extensive experience in developing physics-based software on high-performance computing (HPC) platforms for the study of nano/molecular electronics. We have produced a number of advances in the ability to build large DNA arrays, particularly in 3D. Key advances during the period include methods for self-assembling 3D crystals with multiple components and for making arrays of DNA origami crystals. Significant calculations were performed by the Cui group.

List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

1. F. Mathieu, S. Liao, C. Mao, J. Kopatsch, T. Wang, and N.C. Seeman, Six-Helix Bundles Designed from DNA, NanoLetters 5, 661 -665 (2005).

2. N.C. Seeman, DNA Enables Nanoscale Control of the Structure of Matter, Quart. Rev. Biophys. 38, 363-371 (2005).

3. W.B. Sherman & N.C. Seeman, Design of Low-Stress Nucleic Acid Nanotubes, Biophys. J., 90, 4546-4557 (2006).

4. J. Zheng, P.E. Constantinou, C. Micheel, A.P. Alivisatos, R.A. Kiehl & N.C. Seeman, 2D Nanoparticle Arrays Show the Organizational Power of Robust DNA Motifs, NanoLetters 6, 1502-1504 (2006).

5. A.V. Garibotti, S.M. Knudsen, A.D. Ellington & N.C. Seeman, Functional DNAzymes Organized into 2D Arrays, NanoLetters 6, 1505-1507 (2006).

6. P.E. Constantinou, T. Wang, J. Kopatsch, L.B. Israel, X. Zhang, B. Ding, W.B. Sherman, X. Wang, J. Zheng, R. Sha, N. C. Seeman, Double Cohesion in Structural DNA Nanotechnology, Organic and Biomolecular Chemistry 4, 3414-3419 (2006).

7. J.J. Birac, W.B. Sherman, J. Kopatsch, P.E. Constantinou and N.C. Seeman, GIDEON, A Program for Design in Structural DNA Nanotechnology, J. Mol. Graphics & Modeling 25, 470-480 (2006).

8. G. Wu & N.C. Seeman, A Method of Multiplying with DNA, Natural Computing 5, 427-441, (2006).

9. B. Ding & N.C. Seeman, Operation of a DNA Robot Arm Inserted Into a 2D DNA Crystalline Substrate, Science 314, 1583-1585 (2006).

10. H. Zhong & N.C. Seeman, RNA Used to Control a DNA Rotary Machine, NanoLetters 6, 2899-2903 (2006).

11. A.V. Garibotti, S. Liao & N.C. Seeman, A Simple DNA-Based Translation System, NanoLetters 7, 480-483 (2007).

12. A. Kuzuya, R. Wang, R. Sha & N.C. Seeman, Six-Helix and Eight-Helix DNA Nanotubes Assembled from Half-Tubes, NanoLetters 7, 1757-1763 (2007).

13. X. Wang & N.C. Seeman, The Assembly and Characterization of 8-Arm and 12-Arm DNA Branched Junctions, J. Am. Chem. Soc., 129, 8169-8176 (2007).

14. N.C. Seeman, An Overview of Structural DNA Nanotechnology, Mol. Biotech. 37, 246-257 (2007).

15. C. Lin, X. Wang, Y. Liu, N.C. Seeman & H. Yan, Rolling Circle Enzymatic Replication of a Complex Multi-Crossover DNA Nanostructure, J. Am. Chem. Soc., 129, 14475-14481 (2007).

16. W. Liu, X. Wang, T. Wang, R. Sha & N.C. Seeman, A PX DNA Triangle Oligomerized Using a Novel Three-Domain Motif, NanoLett 8, 317-322 (2008).

17. P.S. Lukeman, M. Stevenson & N.C. Seeman, Morphology Change of Calcium Carbonate in the Presence of Polynucleotides, Cryst. Growth & Design 8, 1200-1202 (2008).

18. Y. Liu, R. Wang, L. Ding, R. Sha, P.S. Lukeman, J. W. Canary & N.C. Seeman, Thermodynamic Analysis of Nylon Nucleic Acids, ChemBioChem 9, 1641-1648 (2008).

19. Y. Liu, R. Sha, R. Wang, L. Ding , J.W. Canary, & N.C. Seeman, 2',2'-Ligation Demonstrates the Thermal Dependence of DNA-Directed Positional Control, Tetrahedron 64, 9417-8422 (2008).

20. Y. Liu, A. Kuzuya, R. Sha, J. Guillaume, R. Wang, J.W. Canary & N.C. Seeman, Coupling Across a DNA Helical Turn Yields a Hybrid DNA/Organic Catenane Doubly Tailed with Functional Termini, J. Am. Chem. Soc. 130, 10882-10883 (2008).

21. J. Zheng, P.S. Lukeman, W.B. Sherman, C. Micheel, A. P. Alivisatos, P.E. Constantinou & N.C. Seeman, Metallic Nanoparticles Used to Estimate the Structural Integrity of DNA Motifs, Biophysical Journal 95, 3340-3348 (2008).

22. B. Chakraborty, R. Sha & N.C. Seeman, A DNA-Based Nanomechanical Device with Three Robust States, Proc. Nat. Acad. Sci. (USA) 105, 17245-17249 (2008).

23. C. Lin, S. Rinker, X. Wang, Y. Liu, N. C. Seeman & H. Yan, In Vivo Cloning of Artificial DNA Nanostructures, Proc. Nat. Acad. Sci. (USA) 105, 17626-17631 (2008).

24. H. Gu, J. Chao, S.J. Xiao & N.C. Seeman, Dynamic Patterning Programmed by DNA Tiles Captured on a DNA Origami Substrate, Nature Nanotech. 4, 245-249, DOI 10.1038/NNANO.2009.5 (2009).

25. T. Omabegho, R. Sha & N.C. Seeman, A Bipedal DNA Brownian Motor with Coordinated Legs, Science 324, 67-71 (2009).

26. C. Liu, N. Jonoska & N.C. Seeman, Reciprocal DNA Nanomechanical Devices Controlled by the Same Set Strands, NanoLetters 9, 2641-2647 (2009).

27. C.H. Spink, L. Ding, Q. Yang, R.D. Sheardy & N.C. Seeman, Thermodynamics of Forming a Parallel Holliday Crossover, Biophys. J. 97, 528-538 (2009).

28. R. Wang, W. Liu & N.C. Seeman, Prototyping Nanorod Control: A DNA Double Helix Sheathed within a DNA 6-Helix Bundle, Chem. &. Biol. 16, 862-867 (2009).

29. J. Zheng, J.J. Birktoft, Y. Chen, T. Wang, R. Sha, P.E. Constantinou, S.L. Ginell, C. Mao, & N.C. Seeman, From Molecular to Macroscopic via the Rational Design of a Self-Assembled 3D DNA Crystal, Nature 461, 74-77 (2009).

30. G. Wu, N. Jonoska & N.C. Seeman, Construction of a DNA Nano-Object Directly Demonstrates Computation, Biosystems 98, 80-84 (2009) DOI: 10.1016/j.biosystems.2009.07.004.

31. J.O. Jensen, H.L. Cui, R.J. Hwu, and D.L. Woolard Ed, “Terahertz for military and security applications VI”, Proceedings of SPIE, Vol. 6949, 2008.

32. M.Q. Weng, M.W. Wu, and H.L. Cui “Spin relaxation in n-type GaAs quantum wells with transient spin grating”, Journal of Applied Physics, 103, 063714 (2008).

33. X.Y. Huang, B. Rosen, and H.L. Cui, “Photonic Bands in Frequency Dependent Media”, to appear in IEEE Journal of Sensors, 2009.

34. N.J. Horing, S.Y. Liu, V.V. Popov, and H.L. Cui, “TUNABLE GRID GATED DOUBLE-QUANTUM-WELL FET TERAHERTZ DETECTOR”, International Journal of High-Speed Electronics and Systems, 18, 147 (2008).

35. N.J. Horing and H.L. Cui, “SURFACE-PLASMON-RESONANCE BASED OPTICAL SENSING”, International Journal of High-Speed Electronics and Systems, 18, 71 (2008).

Number of Papers published in peer-reviewed journals: 35.00

(b) Papers published in non-peer-reviewed journals or in conference proceedings (N/A for none)

1. N.C. Seeman and P.S. Lukeman, Nucleic Acid Nanostructures, Reports on Progress in Physics 68, 237-270 (2005).

2. N.C. Seeman, B. Ding , S. Liao , T. Wang, W.B. Sherman, P.E. Constantinou, J. Kopatsch, C. Mao, R. Sha, F. Liu, H. Yan & P.S. Lukeman, Experiments in Structural DNA Nanotechnology: Arrays and Devices , Proc. SPIE; Nanofabrication: Technologies, Devices and Applications 5592, 71-81 (2005).

3. N.C. Seeman, From Genes to Machines: DNA Nanomechanical Devices, Trends in Biochemical Sciences 30, 119-125 (2005).

4. N.C. Seeman. Structural DNA Nanotechnology: An Overview. Methods in Molecular Biology 303: Bionanotechnology Protocols, Editors, Sandra J. Rosenthal and David W. Wright, Humana Press, Totowa, NJ, pp. 143-166 (2005).

5. R. Sha, X. Zhang, S. Liao, P.E. Constantinou, B. Ding, T. Wang, A.V. Garibotti, H. Zhong, L.B. Israel, X. Wang,, G. Wu, B. Chakraborty, J. Chen, Y. Zhang, C. Mao, H. Yan, J. Kopatsch, J. Zheng, P.S. Lukeman, W.B. Sherman, N.C. Seeman., Motifs and Methods in Structural DNA Nanotechnology, Proc. Intl. Conf. Nanomaterials, NANO 2005, July 13-15, 2005, Mepco Schlenk Engineering College, Srivakasi, India, V. Rajendran, ed., pp. 3-10 (2005).

6. R. Sha, X. Zhang, S.Liao, P.E. Constantinou, B. Ding, T. Wang, A.V. Garibotti, H. Zhong, L.B. Israel, X. Wang, G. Wu, B. Chakraborty, J. Chen, Y. Zhang, H. Yan, Z. Shen, W. Shen, P. Sa-Ardyen, J. Kopatsch, J. Zheng, P.S. Lukeman, W.B. Sherman, C. Mao, N. Jonoska & N.C. Seeman, Structural DNA Nanotechnology: Molecular Construction and Computation, Unconventional Computation: Proceedings of UC 2005, 4th International Conference, Sevilla Spain, Oct 2005. Lecture Notes in Computer Science 3699, C.S; Calude, M.J. Dinneen, G. Paun, M.J. Perez-Jimenez, G. Rozenberg, eds., 20-31 (2005).

7. N.C. Seeman, The Challenge of Structural Control on the Nanoscale: Bottom-Up Self-Assembly of Nucleic Acids in 3D, Int. J. Nanotech. 2, 348-370 (2005).

8. C. Mao, P.E. Constantinou, F. Liu, Y. Pinto, J. Kopatsch, P.S. Lukeman, T. Wang, B. Ding, H. Yan, J.J. Birktoft, R. Sha, H.Zhong, L. Foley, L.A. Wenzler, R. Sweet, M. Becker and N.C. Seeman, The Design of Self-Assembled 3D DNA Networks, Proc. Intl. Symp. on Nanoscale Devices, Materials, and Biological Systems, 206th Meeting of the Electrochemical Society, Honolulu, PV 2004-XX, Editors: M. Cahay, M. Urquidi-Macdonald, S.Bandyopadhyay, P. Guo, H. Hasegawa, N. Koshida, J.P. Leburton, D.J., Lockwood, S. Seal, and A. Stella., vol. 13, 509-520 (2005).

9. N.C. Seeman, Nanotechnology and the Double Helix, Scientific American Reports, 30-39, September issue (2007).

10. N.C. Seeman, Synthetic Single-Stranded DNA Topology, Applications of Knot Theory, D. Buck & E. Flapan, Eds, Am. Math. Soc. Proc. Symp. Applied. Math. 66 121-153 (2009).

11. N.C. Seeman, The Perils of Polynucleotides Revisited, in Algorithmic Processes, A. Condon, D. Harel, J.N. Kok, A. Salomaa and E. Winfree, eds., Springer, pp. 205-214 (2009).

Number of Papers published in non peer-reviewed journals: 10.00

(c) Presentations

Engineering a DNA World, Pasadena, 2005.
National Acad. Sciences Workshop on Molecular Manufacturing, Washington DC, 2005.
RSC Conference on Chemical Nanoscience and Nanotechnology, Nottingham, 2005.
Fourth International Symposium on Chemical Biophysics, Toronto, 2005.
Nobel Workshop on Fundamentals of Biomolecular Function, Coimbra, 2005.
Turing Days Symposium, Istanbul Bilgi Üniversitesi, Istanbul, 2005.
American Chemical Society, MARM, Piscataway, NJ, 2005.
11th Conference on DNA-Based Computing (tutorial), London, Ont., 2005.
NANO 2005, Sivakasi, Tamil Nadu, 2005.
Seventh Beckman Symposium, Irvine, CA, 2005.
New York Structural Biology Discussion Group, Cold Spring Harbor, 2005.
15th IUPAB and 5th EBSA Conference, Montpellier, 2005.
Ninth International Conference on Environmental Mutagens, San Francisco, 2005.
British Association for the Advancement of Science Festival, Dublin, 2005.
Biocomputers 2005, Seoul, 2005.
Third COE Symposium on Human Friendly Materials Based on Chemistry, Tokyo, 2005.
Fourth Conference on Unusual Computation, Sevilla, 2005.
Fifth Virtual Conference on Genomics and Bioinformatics, Arlington, VA, 2005.
American Vacuum Society, Boston, 2005.
NSF Workshop on Opportunities of Nanoscience to Energy, Arlington, VA, 2005.
Molecular Biology Society of Japan, Fukuoka, 2005.
NYU-Penn Soft Matter Workshop, New York, 2006.
Structure by Design, Biophysical Society, Salt Lake City, 2006.
Workshop on Sensing Biomolecular Architectures, Charlottesville, 2006.
Genomes to Systems Conference, Manchester, 2006.
New York Nanoscience Discussion Group, New York, 2006.
DNA-Based Nanoscale Integration, Jena, 2006.
89th Canadian Chemistry Conference, Halifax, 2006.
12th Conference on DNA-Based Computing (tutorial), Seoul, 2006.
Canadian Society of Microbiology/Genetics Society of Canada, London, Ontario, 2006.
Fifth Workshop on Future Trends in Microelectronics, Aghia Pelagia, Crete, 2006.
International Conference on Nanoscience and Nanotechnology, Brisbane, 2006.
NSF Workshop on Cyber Infrastructure in Materials Science, 2006.
International Roundtable on Nucleosides Nucleotides and Nucleic Acids-XVII, Bern, 2006.
Second Symposium on Semiconductor Wires, Lund (Keynote + Tutorial), 2006.
Complex Molecular Architectures on Surfaces, Bonn, 2006.
Seventh Dartmouth Symposium on Nanomaterials, 2006.
Nano: The Future is Here, Giessen, 2006.
NSF Workshop on the Computational World View and the Sciences, Princeton, 2006.
Advanced Architectures for Biological Agent Detection & Discrimination, Hoboken, 2007.
Trends in Nanoscience, Kloster Irsee, 2007.
Arthur M. Sackler Symposium on Nanomaterials, Washington DC, 2007.
Pre-Biotic Chemistry and Early Evolution, Dubrovnik, 2007.
Thirteenth Conference on DNA-Based Computing (tutorial), Memphis, 2007.
Fifteenth Conversation on Biomolecular Stereodynamics, Albany, 2007.
Workshop on Tilings and Self-Assembly, Turku, 2007.
Goddard Symposium, Am. Chem. Soc., Boston, 2007.
Challenges and Opportunities for the Future of Nano and Bio Technologies, Tucson, 2007.
Molecular Foundry-Advanced Light Source User's Meeting, Berkeley, 2007.
Second International Symposium on Bio-Inspired Engineering, Dead Sea, 2007.
Workshop in NSF Nanoelectronics, Arlington, VA, 2007.
NYNBIT Technical Meeting, Utica, 2007.
Nucleic Acid Science: The Excitement of Discovery, Chemische Gesellschaft Zurich, 2007.
Knotting Mathematics and Art, Tampa, 2007.
DOE Biomolecular Materials Meeting, Warrenton, VA, 2007.
CIFAR Nanoelectronics Program Meeting, Vancouver, 2007.

Materials Research Society, Boston, 2007.
Workshop on Algorithmic Bioprocesses, Leiden, 2007.
Short Course on Applications of Knot Theory, American Math. Soc., San Diego, 2008.
Impact of Nucleic Acid Nanostructure on Function, Bangalore, 2008.
William H. Nichols Lecture, White Plains, NY 2008.
Materials Research Society, San Francisco, 2008.
New York Nanoscience Discussion Group, 2008.
Office of Naval Research, DNA Nanofabrication Workshop, Washington, DC, 2008.
American Chemical Society, MARM, Queens, NY, 2008.
Neville R. Kallenbach 70th Birthday Symposium, New York, 2008.
Molecular Frontiers Symposium, Stockholm, 2008.
Fourteenth Conference on DNA-Based Computing (tutorial), Prague, 2008.
Third CIMTEC Conference on Smart Materials, Structures and Systems, Acireale, 2008.
International Symposium on Spectral Sensing Research, Hoboken, 2008.
Third Int'l Symposium on Macrocyclic and Supramolecular Chemistry, Las Vegas, 2008
DSRC Workshop, Harvard, Cambridge, 2008.
Nanotides Symposium, Düsseldorf, 2008.

Number of Presentations: 71.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts): 0

Peer-Reviewed Conference Proceeding publications (other than abstracts):

1. X. Huang, B. Rosen, and H.L. Cui "Photonic Band Modification by Molecular Resonance", ISSSR 2008.

2. Xiaoyang Huang, Duan Zhang, Bernard Rosen, and Hong-Liang Cui, "TERAHERZ WAVE PROPAGATION IN TWO-DIMENSIONAL PHOTONIC CRYSTAL WITH EMBEDDED MOLECULES", NANO-DDS 2009.

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts): 2

(d) Manuscripts

Number of Manuscripts: 0.00

Number of Inventions:

Graduate Students

NAME	PERCENT SUPPORTED
Hong Zhong	1.00
Risheng Wang	0.50
Wenyan Liu	1.00
Baoquan Ding	0.25
Jianping Zheng	0.25
Alejandra Garibotti	0.25
Jie Xu	0.50
Jing Xie	0.50
FTE Equivalent:	**4.25**
Total Number:	**8**

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Xiaoyang Huang	0.50
Greg Racine	0.50
Bernard Rosen	1.00
Jiwen Zheng	0.25
Ruojie Sha	0.10
FTE Equivalent:	**2.35**
Total Number:	**5**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: .....

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:.....

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:.....

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale): .....

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering: .....

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense .....

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: .....

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME
Hong Zhong
Alejandra Garibotti
Baoquan Ding
Total Number: 3

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

5 **A Nucleic Acid-Based Nanorobotic System**

Patent Filed in US? (5d-1) Y

Patent Filed in Foreign Countries? (5d-2) N

Was the assignment forwarded to the contracting officer? (5e) Y

Foreign Countries of application (5g-2):

5a: William B. Sherman

5f-1a: New York University

5f-c: 100 Washington Square East

New York NY 10003

5a: Nadrian C. Seeman

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5f-c: 100 Washington Square East

New York NY 10003

5 **A Polynucleic Acid Nanomechanical Device Controlled by Hybridization Topology**

Patent Filed in US? (5d-1) Y

Patent Filed in Foreign Countries? (5d-2) N

Was the assignment forwarded to the contracting officer? (5e) Y

Foreign Countries of application (5g-2):

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New York NY 10003

5a: Xiaoping Zhang

5f-1a: New York University

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5a: Nadrian C. Seeman

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5f-c: 100 Washington Square East

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5a: Zhiyong Shen

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5 **A Polynucleotide Nanomechanical Device that Acts as an Artificial Ribosome and Translates DNA Signals into Polymer Assembly Instructi**

Patent Filed in US? (5d-1) Y

Patent Filed in Foreign Countries? (5d-2) N

Was the assignment forwarded to the contracting officer? (5e) Y

Foreign Countries of application (5g-2):

5a: James W. Canary

5f-1a: New York University

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5f-1a: New York University

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5a: Nadrian C. Seeman

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5a: Shiping Liao

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New York NY 10003

5 **Nucleic Acid-Nylon Ladder Polymers**

Patent Filed in US? (5d-1) Y

Patent Filed in Foreign Countries? (5d-2) N

Was the assignment forwarded to the contracting officer? (5e) Y

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5a: Philip S. Lukeman

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5a: Nadrian C. Seeman

5f-1a: New York University

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5 **Nylon Ribopolynucleosides**

Patent Filed in US? (5d-1) Y

Patent Filed in Foreign Countries? (5d-2) N

Was the assignment forwarded to the contracting officer? (5e) Y

Foreign Countries of application (5g-2):

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5a: Nadrian C. Seeman

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5f-c: 100 Washington Square East

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5a: Ruojie Sha

5f-1a: New York University

5f-c: 100 Washington Square East

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5a: Yu Liu

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5f-c: 100 Washington Square East

New York NY 10003

5a: Liang Ding

5f-1a: New York University

5f-c: 100 Washington Square East

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5 **Polygonal Nanostructures of Polynucleic Acid Multi-Crossover Molecules and Assembly of Lattices Based on Double Crossover Cohesion**

Patent Filed in US? (5d-1) Y

Patent Filed in Foreign Countries? (5d-2) N

Was the assignment forwarded to the contracting officer? (5e) Y

Foreign Countries of application (5g-2):

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5a: Lisa B. Israel

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5a: Pamela E. Constantinou

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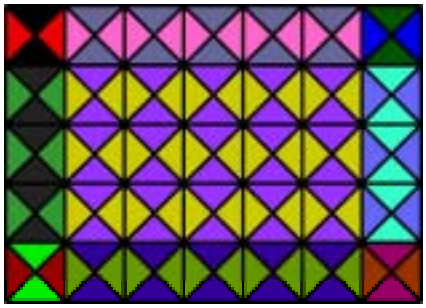
Table of Contents

Key Activities of the Prime Contractor, Nadrian C. Seeman of the Chemistry Department of New York University

The tasks undertaken for this project include: (1) defining and fabricating new DNA-based photonic band-gap wave-guiding structures to facilitate quasi-optical control of signal propagation in integrated molecular/electronic systems; (2) defining and studying new bio-inspired paradigms for establishing electro-optical communication channels and propagating wave control methodologies useful for incorporation into biologically-based devices and components; and (3) defining and, modeling, fabricating and testing hybrid multi-terminal bio-molecular devices that can achieve (a) control and manipulation of signal propagation, and (b) enhanced sensor function, using molecular-level characteristics.

The NYU group focused in area (1) on the construction of two-dimensional DNA arrangements with periodicities that far exceed those that have been reported previously. During the first year, a student, Hong Zhong, worked on this task full time. The approach at that time entailed using a 2D variant of the Yan method[1] for building 2D arrays. We chose to make a 5 x 7 array, as shown on the right. Such an array entails unique long strands on each of the four edges, and strands with multiple use in the central portions, both vertical and horizontal. We designed such a system from DNA parallelograms[2]. We spent quite a lot of time in building the four unique edge strands. They are too long to synthesize directly on the DNA synthesizer, so it is necessary to ligate their components together. They entail ligation of molecules that of necessity contain common elements, and that has led to certain difficulties in the ligation of their components. We have preliminary indications that we have overcome these problems in at least one strand.



A postdoc during that time is worked on the task of attaching gold nanoparticles to DNA lattices. This is a task preliminary to the addition of photonic materials to the DNA lattices.

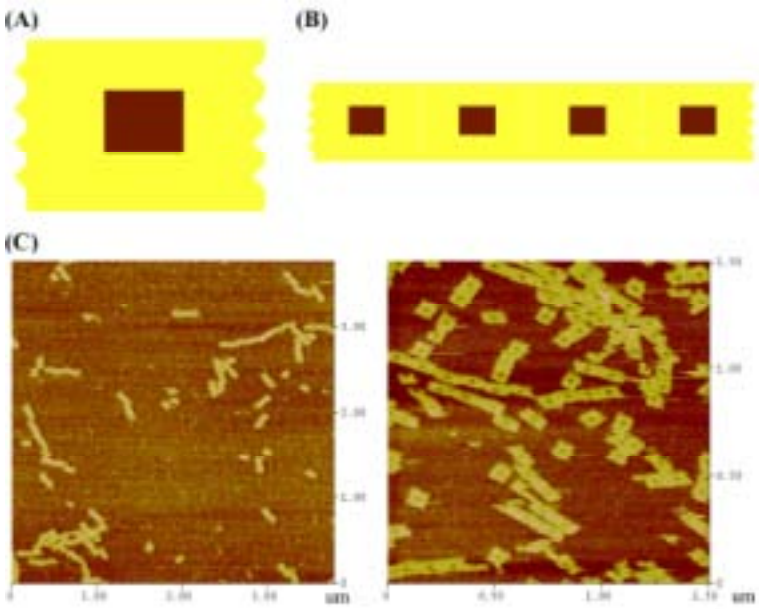
During the second year, we switched from the Yan method to the Rothemund method[3] for building 2D arrays. The components are squares about 100 x 100 nm. We have focused on this approach through the current time in this aspect of the work.

Also during the second year of the project, we were successful in arranging metallic nanoparticles into 2D checkerboard patterns.[4] This work used robust motifs, and the method has been used recently in organizing dyes in 3D crystals, which were achieved later in the project.[5]

A second success during the second year was the organization of functional DNAzymes in 2D arrays.[6] Thus, it is possible to place catalytic activities at specific loci within a 2D crystalline network just through sequence design.

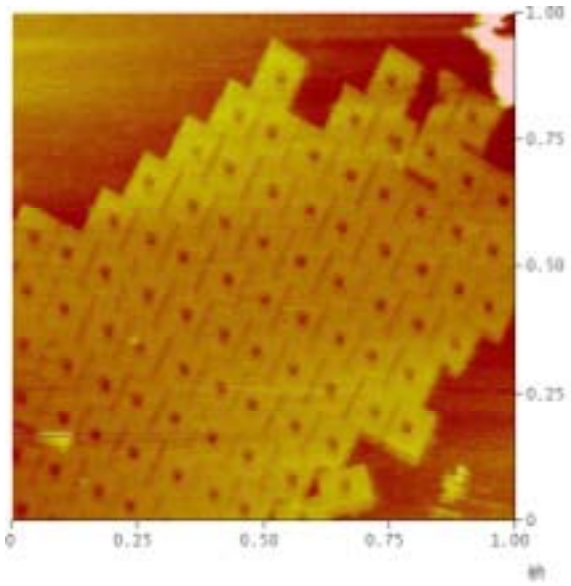
A major achievement during this period is the organization of sequence-dependent DNA-based nanomechanical devices into 2D DNA lattices.[7] This work leads to the capability of being able to change the spatial organization of components in a lattice.

During the third year, we learned in part how to work with the Rothemund arrays. We are quite successful in building up larger structures in one dimension, as seen below but 2D control is more elusive.



One-dimensional origami array. (A) Schematic view of a single B tile for the construction of the 1D array. There are four 'donor' sites in the left edge of the tile B and four 'acceptor' sites at right. The protruding triangles represent four 8 nucleotide sticky ends, which are complimentary to the 'acceptor' sites to the right, specifically. (B) illustrates a linear structure with four tiles. (C) AFM images of the 1D array.

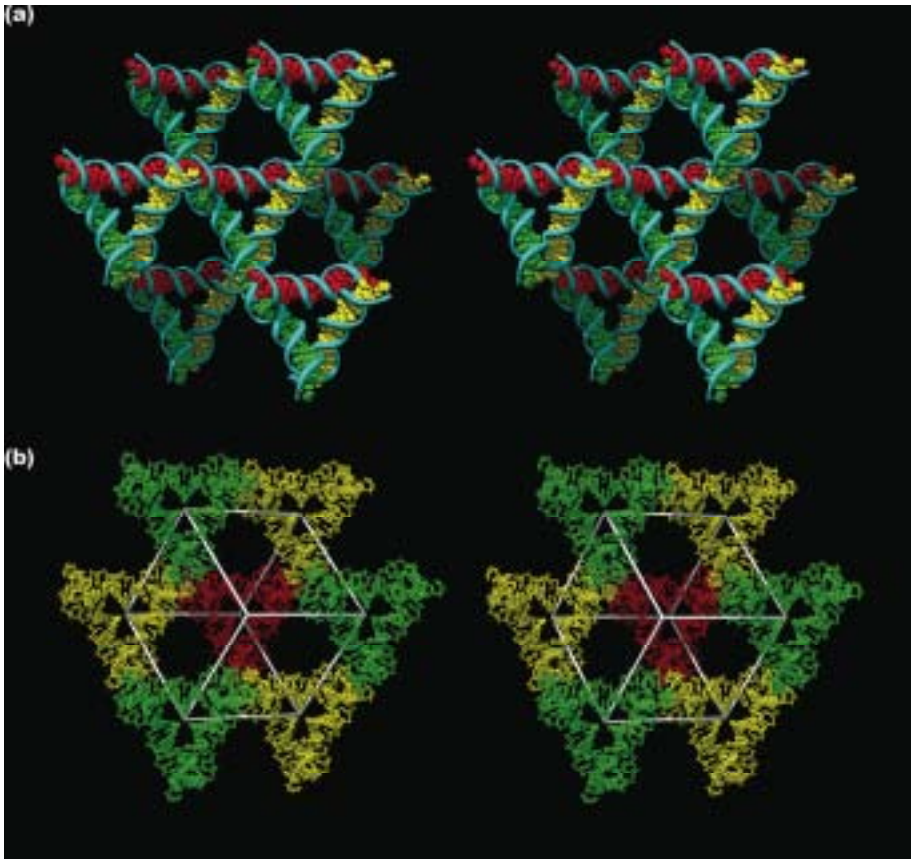
During the fourth year, we were more successful with the 2D Rothemund arrays. This can be seen in the image below.



A recurring problem is that the crystals grow much better in the longitudinal direction. We have a plan to correct that, which is currently undergoing testing.

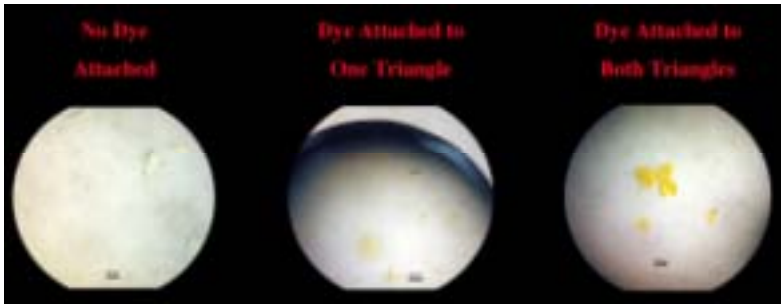
As noted above, we have been very successful in building a variety of designed and self-assembled 3D crystalline arrangements based on tensegrity triangles.[5] A picture of the

molecular structure, established by X-ray crystallography is shown below in stereographic projection.



Designed Crystalline Arrangement. *(a) Surroundings of a Triangle.* This stereoscopic image distinguishes three independent directions by base pair color. The central triangle is flanked by six other triangles. *(b) Rhombohedral Cavity Formed by Tensegrity Triangles.* This stereoscopic image shows seven of the eight triangles that comprise the rhombohedron's corners. The cavity outline is drawn white. The rear red triangle connects through one edge each to the three yellow triangles in a plane closer to the viewer. The yellow triangles are connected through two edges each to two different green triangles that are even nearer the viewer.

We have been able to include more than one molecular species within a crystal. In the image below, we have attached fluorescein dye to 0, 1 or both of the different triangles, which is evident from the colored intensity of the crystals.



Thus, in summary, we have established a number of features of the control of the structure of matter using DNA that have not been described previously. These include the organization of nanoparticles in 2D, the organization of nanomechanical devices in 2D, the organization of DNAzymes in 2D, the longer-distance organization of Rothemund tiles in 1D and 2D and the macroscopic 3D organization of DNA and pendent dyes. All of these advances will serve to build deliberate photonic band gap materials.

People Supported:

Hong Zhong, Graduate Student
Wenyan Liu, Graduate Student
Risheng Wang, Graduate Student
Baoquan Ding, Graduate Student (in part)
Alejandra Garibotti, Graduate Student (in part)
Jianping Zheng, Graduate Student (in part)
Jiwen Zheng, Post-doc (in part)
Ruojie Sha, Sr. Res. Assoc. (in part)

Activities on the Sub-Contractor, Hong-Liang Cui, Stevens Institute of Technology Final Report

US Army-NYU Project

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November 15, 2009

People Supported:

Bernard Rosen, Research Professor
Greg Recine, Research Assistant Professor (partial support)
Xiaoyang Huang, Postdoctoral Associate (partial support)
Jie Xu, Graduate Student (partial support)
Jing Xie, Graduate Student (partial support)

Publications:

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2. M.Q. Weng, M.W. Wu, and H.L. Cui "Spin relaxation in n-type GaAs quantum wells with transient spin grating", Journal of Applied Physics, **103**, 063714 (2008).
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Media", to appear in IEEE Journal of Sensors, 2009.
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5. N.J. Horing, S.Y. Liu, V.V. Popov, and H.L. Cui, "TUNABLE GRID GATED DOUBLE-QUANTUM-WELL FET TERAHERTZ DETECTOR", International Journal of High-Speed Electronics and Systems, **18**, 147 (2008).
6. N.J. Horing and H.L. Cui, "SURFACE-PLASMON-RESONANCE BASED OPTICAL SENSING", International Journal of High-Speed Electronics and Systems, **18**, 71 (2008).
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Technical Report:

Part I: 2D Photonic Crystal Propagation Codes Incorporating Conductive Losses and Frequency-Dependent Materials

I. Background

The control and detection of electromagnetic(EM) radiation has been of the cornerstones of technology for more than a century. First proposed decades ago, photonic crystals are a class of materials developed for the control of light propagation. The crystals are, for the most part, man-made, microscopically periodic materials. The spatial periodicity is on the scale of the wavelength of the radiation to be controlled. Several interesting devices using biologically-active molecules embedded in a photonic crystals structure have been proposed [1,2] for the control and detection of terahertz radiation. The embedding lattice is itself notable, namely, it consists of strands of artificially produced DNA. The molecules may possibly be attached to the DNA by small metallic(gold) particles.

The algorithms described here are designed for the investigation of the propagation of electromagnetic waves in such a lattice. There is a periodicity in optical properties in the two directions perpendicular to that of the strands of DNA and it is assumed that the material is uniform in the direction parallel to the strands. In addition to losses by reflection, the EM waves can suffer absorption by the DNA material, by the molecules, and by the gold particles. Furthermore, the frequency dependence of the optical response of the active medium is key to the operation of the devices of interest.

In previous theoretical work involving photonic crystals built with DNA carried out in this laboratory, the MPB program[3] developed at MIT was used to study the optical behavior. The design of MPB does not include provisions for the incorporation of absorption or of frequency-dependent material. The algorithms presented here can take both effects into account.

The intended applications of these results is to arrangements in which EM waves of specified frequencies originate in controllable sources and then impinge on photonic crystals of finite thickness. Besides the reflections that occur on entrance and exit because of impedance mismatch, the material itself may attenuate the signal by a combination of reflection and absorption and these properties are the ones to be investigated via the algorithms presented here. Once the propagation constant (possibly complex) of a mode has been determined, one can use the well-known procedures of scattering theory to determine the appropriate combinations of forward and reflected waves.

In the following section we present the basic theory of the algorithms, first for the "TE" case, for which the electric field is taken to be parallel to the direction of the DNA strands, and perpendicular to the plane of propagation and then the "TM" case where now the magnetic induction field is parallel to the strands. Some typical results are illustrated further on.

II. FORMULATION

A. Physical Specification

The plane of propagation is taken to be the x-y plane. Each of the fields is expressed as a plane wave,

$\exp(ik \cdot r - i\omega t)$,

multiplied by a doubly-periodic function of x and y. Here, the spatial periodicities are Lx and Ly, and the corresponding Fourier space is characterized by K_{0x} =2π /Lx and K_{0y} =2π /Ly. The vector **k** (=(k_x, k_y)), the propagation vector, equals k{cos(_),sin(_)}, where k=|**k**| is the ***wave number***. In the TE case, for example, the electric field would have the form:

$$E_z = \sum_{mx,my} \alpha[mx, my] \exp[i(m_x K_{0x} x + m_y K_{0y} y)]$$

exp[i **k** · **r** - i _ t]. (Field-1)

Instead of B_x and B_y we use the components of B parallel and perpendicular to **k**:

$$B_{\|} = \sum_{mx,my} \beta[mx, my] \exp[i(m_x K_{0x} x + m_y K_{0y} y)]$$

exp[i **k** · **r** - i _ t]. (Field-2)

$$B \perp = \sum_{mx,my} \gamma[mx, my] \exp[i(m_x K_{0x} x + m_y K_{0y} y)]$$

exp[i **k** · **r** - i _ t]. (Field-3)

These forms are to be inserted into the Maxwell equations and the common factor exp[i k · r + i _ t] is canceled out after the differentiations are performed. Following this, Fourier analysis is carried out by multiplying each equation by

$\exp[-i(l_x K_{0x} x + l_y K_{0y} y)]$

and then integrating them over a "unit cell"

[0<= x < Lx , 0 <= y < Ly]..

The essence of photonic propagation, as opposed to propagation in a uniform medium, is the variation of _ over a unit cell. As a result of the integrations indicated above, the Fourier components of the dielectric function, ℳ, will emerge and be found to couple the coefficients _[m_x, m_y] belonging to different values of m_x and m_y .

As indicated above, it is useful to use the components of the fields along and perpendicular to the wave vector. The unit vector $e_{\|}$ taken parallel to the direction of propagation, e_z is perpendicular to the x-y plane, and $e_{\perp}$ lies in that plane but is perpendicular to $e_{\|}$. In that order they form a right-handed triad.

B. TE (photonics TM) Case

The z component of the Maxwell-Ampere Law is

$$e_z \cdot (\partial_t \varepsilon_1 E - c^2 \nabla \times B) = 0$$

where ε_1 is $\varepsilon/\varepsilon_0$, μ is taken to be μ_0,c is the speed of light in vacuum, and $\partial_t \equiv \frac{\partial}{\partial t}$.

Performing the resolution of **B** yields

$$\frac{1}{c^2}\partial_t \varepsilon_1 E_z + (\partial_{\|} B_{\perp} - \partial_{\perp} B_{\|}) = 0 \ , \qquad \text{(TE-1)}$$

where the symbols $\partial_{\|} \equiv e_{\|} \cdot \nabla$, and $\partial_{\perp} \equiv e_{\perp} \cdot \nabla$ have been introduced..

These operators are ultimately to be interpreted in terms of the expressions for the fields (Field 1, 2, 3) given above. For example, $\partial_{\perp}$ will become

$$i(m_x K_{0x} \sin(\theta) - m_x K_{0y} \cos(\theta)),$$

where cos(_)= x/|r|. The product will be a convolution sum that can be written as a matrix of the Fourier coefficients of ε_1 acting on a vector of the Fourier coefficients, ♋[mx, my], of E_z. Note that operating with $\partial_{\|}$ on the fields involves a term with k in addition to those with K_{0x} and/or K_{0y}.

Faraday's Law

$$\partial_t B + \nabla \times E = 0$$

can be resolved into the perpendicular and parallel components as

$$\partial_t B_{\perp} + \partial_{\|} E_z = 0 \qquad \text{(TE-2)}$$

and

$$\partial_t B_{\|} - \partial_{\perp} E_z = 0 \qquad \text{(TE-3)}$$

The last equation does not contain the wave number, k, and hence cannot be used directly to obtain an eigenvalue equation for it. One proceeds as follows:

Apply ∂_t to Eq.(TE-1), interchange ∂_t and $\partial_{\perp}$ in the last term and substitute (TE-3) for $\partial_t B_{\|}$ to get

$$\frac{1}{c^2}\partial_t \partial_t E_z - (-\partial_{\|} \frac{1}{c} \partial_t B_{\perp} + \partial_{\perp} \partial_{\perp} E_z) = 0 \quad \text{(TE-1')}$$

Eqs (TE-1') and (TE-2) can be written in symbolic matrix form .

$$\begin{bmatrix} i\partial_{\|} & -1 \\ \frac{1}{c^2}\partial_t^2\varepsilon_1 - \partial_{\perp}^2 & i\partial_{\|} \end{bmatrix} \begin{bmatrix} E_z \\ -i\frac{1}{c}\partial_t B_{\perp} \end{bmatrix} = 0$$

Insertion of the Fourier expansions Eqs.(Field 1, 2, 3) leads directly to the eigenvalue equation for k,.

$$\text{Determinant} \begin{bmatrix} -KA-k & -1 \\ -(\omega/c)^2\tilde{\varepsilon} - KP^2 & -KA-k \end{bmatrix} = 0$$

(TE-Eigen)

The vector of fields is formed from the Fourier coefficients ♋ and ♌. KA and KP are block diagonal matrices(see below) as is"-1", while $\tilde{\varepsilon} = \tilde{\varepsilon}[l_x, l_y; m_x, m_y]$ is the matrix of Fourier coefficients of ε_1. It is necessary, of course, to truncate the infinite matrices, choosing, say, [-Nx, Nx] and [-Ny, Ny] to be the ranges of m_x and m_y, respectively, in the Fourier expansions given in Eqs(Field 1,2,3)). Each block in (TE-Eigen) is of dimension (2 Nx +1) (2 Ny + 1) and the mapping of $[l_x, l_y; m_x, m_y]$ to the two-dimensional form of (TE-Eigen) is

row index= $(l_y + \text{Ny})(2\,\text{Nx} + 1) + l_x + \text{Nx} + 1$,

column index = $(m_y + \text{Ny})(2\,\text{Nx} + 1) + m_x + \text{Nx} + 1$.

The KA and KP matrices are given by

$$\text{KA}[l_x, l_y; m_x, m_y] =$$
$$(l_x K_{0x}\cos(\theta) + l_y K_{0y}\sin(\theta))\ \delta_{lx,mx}\,\delta_{ly,my}$$

$$\text{KP}[l_x, l_y; m_x, m_y] =$$
$$(l_x K_{0x}\sin(\theta) - l_y K_{0y}\cos(\theta))\ \delta_{lx,mx}\,\delta_{ly,my}$$

where $\delta_{lx,mx}$ and $\delta_{ly,my}$ are Kronecker deltas.

C. TM (photonics TE) Case

The TM case is handled in much the same way except that $D = \varepsilon E$ plays a slightly more complicated role.

Once again, we use the Faraday's law, this time for the z component of B

$$\partial_t B_z - \partial_{\|} E_{\perp} + \partial_{\perp} E_{\|} = 0 \qquad \text{(TM 1)}$$

The parallel and perpendicular components of the Maxwell-Ampere Law are

$$\frac{1}{c}\partial_t \varepsilon_1 E_\perp - \partial_\parallel B_z = 0 \qquad \text{(TM 2)}$$

$$\frac{1}{c}\partial_t \varepsilon_1 E_\parallel - \partial_\perp B_z = 0 \qquad \text{(TM 3)}$$

Proceeding as before, one obtains

$$\varepsilon_1 \frac{1}{c^2}\partial_t \partial_t B_z + (-\varepsilon_1 \partial_\parallel \varepsilon_1^{-1} \frac{1}{c}\partial_t E_\perp + \varepsilon_1 \partial_\perp \varepsilon_1^{-1} \partial_\perp B_z) = 0$$

Again, in symbolic form, there results:

$$\begin{bmatrix} -KA - k & -1 \\ -(\omega/c)^2 \tilde{\varepsilon} - \Pi & -\Lambda - k \end{bmatrix} \begin{bmatrix} B \\ -\omega/c\, D_\perp \end{bmatrix} = 0 \quad \text{(TM-4)}$$

where

$\Pi = \tilde{\varepsilon} KP \tilde{\varepsilon}^{-1} KP$,

and

$\Lambda = \tilde{\varepsilon} KA \tilde{\varepsilon}^{-1}$.

The eigenvalue equation for k follows once again from the necessity that determinant of the matrix in Eq.(TM-4) vanish for the existence of a non-trivial solution.

D. Inclusion of Conductivity

As indicated above the inclusion of the effects of conductivity(♦) on the propagation of waves in a photonic crystal is required by the application. For fields with the steady-state time dependence it is sufficient to make the replacement of ℳ by the frequency dependent

$$\varepsilon_1' = \varepsilon_1 + \frac{i\sigma}{\omega \varepsilon_0}.$$

III. Eigenvalues of Uncoupled Modes

The TE mode field configuration is considered here.

Should a unit cell be filled completely with one material then $\tilde{\varepsilon}$ is a multiple of the identity matrix. The Fourier modes would be decoupled and the eigenvalue equation for any one mode would be given by (**det** stands for determinant)

$$\det \begin{bmatrix} -ka-k & -1 \\ kp^2 - \bar{\varepsilon}_1 (\omega/c)^2 & -ka-k \end{bmatrix} = 0$$

where ka and kp are the elements of KA and KP for the values $l_x (= m_x), l_y (= m_y)$ while $\bar{\varepsilon}_1$ is the average value of ε_1 over one cell of the lattice.

The eigenvalues of k are

$$k_{\pm} = -ka \pm \sqrt{\bar{\varepsilon}_1 (\omega/c)^2 - kp^2}$$

Except for the special case, $l_x = l_y = 0$, and for ◆ small , k has a constant real part, -ka, and an imaginary part that decreases with increasing ◆. When $\bar{\varepsilon}_1 (\omega/c)^2 \geq kp^2$, k becomes purely real..

If the dispersion relation just given is written as

$(k + ka)^2 + kp^2 = \bar{\varepsilon}_1 (\omega/c)^2$,

it resembles that for modes in a waveguide. By analogy, the frequency region for which $\bar{\varepsilon}_1 (\omega/c)^2 < kp^2$ will be referred to as ***cutoff*.**

IV. APPLICATIONS

The presence of molecules possessing a resonant frequency in the neighborhood of a cutoff region of the photonic crystal can significantly modify the k- characteristics of the lattice from those in the absence of the molecules. In particular, the magnitude of the reflection of waves in the frequency range below cutoff can be lowered because of the raising of the index of refraction by the molecules. This decrease in the attenuation takes place despite the added absorption due to the molecules.

To illustrate this effect we carried out a computer simulation was carried out in which the dimensions of the unit cell were Lx=43 micros and Ly=110 microns. In each cell half was filled with material for which ε_1=1.33 and the other half with either the molecules described below or with air. The split in properties took place halfway across the unit cell in the x direction, which was the direction of propagation.

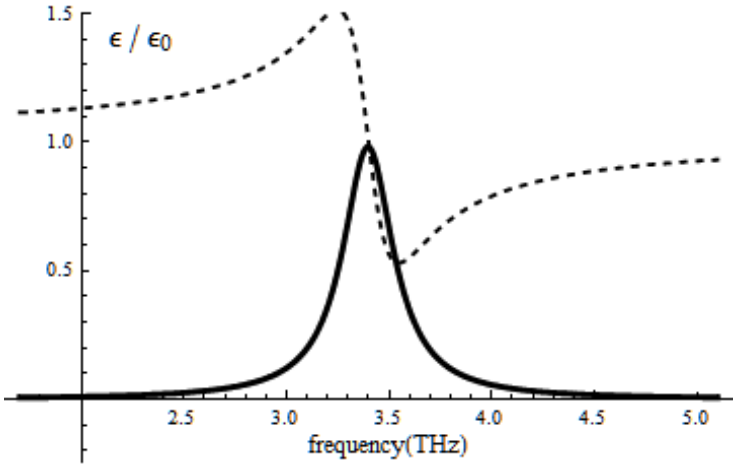

Figure 1. The real (dashed curve) and imaginary(solid curve) parts of the dielectric response ε_1

In Fig. 1 the relative dielectric function, ε_1, according to the Drude model

$$\varepsilon_1 = 1 + \frac{\omega_p^2}{\omega_R^2 - \omega^2 - i\gamma\omega}$$

is shown for the parameters $\omega_p/2\pi = 1.0$, $\omega_R/2\pi = 3.4$ $\gamma/2\pi = 0.3$, all in THz. The value of ω_p is somewhat unrealistically high but chosen for illustrative purposes.

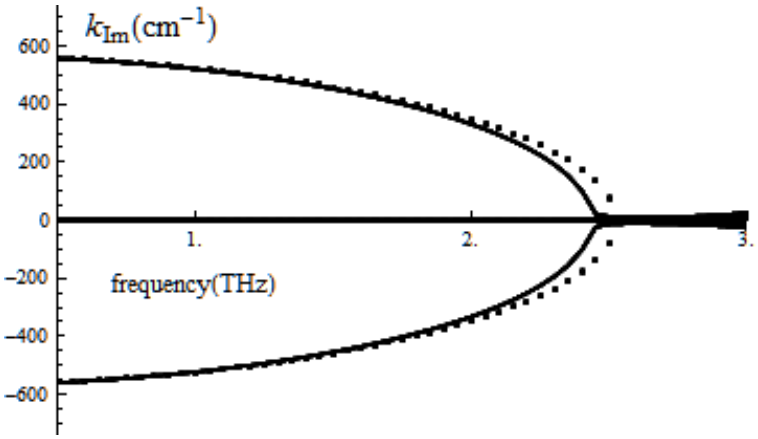

Figure 2. Alteration of reflection in photonic crystal propagation due to resonant molecules.

The alteration of the absorption (reflection) coefficient by the presence of such a molecular resonance is illustrated in Fig 2. More precisely, k_I, the imaginary part of k, is plotted as a function of frequency both for no molecules (dashed curve) and in the presence of molecules (solid curve) in half the cell. The decrease in k_I for the waveguide-

like mode below the molecular resonance is apparent.

Below about 2.5 THZ the wave is attenuated, decaying as $\exp(-k_I x)$ because of reflection; this is the cutoff region described in the previous section. Because of the increased index of refraction due to the molecules, the mode "comes out of cutoff" at a lower frequency.

Schematically, for the parameters stated above, given a source of radiation with a frequency at 2.4 THz incident on one face the crystal, and a detector at the opposite side, the presence of molecules in sufficient concentration could cause a substantial rise in the detected signal.

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Part II Photonic BioSensors

Electromagnetic wave propagation in two-dimensional photonic crystal is investigated. The influence of metal such as gold on the propagation characteristics in the visible region is considered. Gold shows to have impact on the lower frequencies. When go to the Teraherz regime, molecules are embedded to the unit cell to see its influence on the propagation behavior. It shows that by selecting proper molecules, the cutoff frequency is shifted. However, DNA frame also plays a big role. Based on the calculation, DNA frame is seen not to be a neutral background, instead it brings loss in the low frequency range. To summarize, the investigation of electromagnetic wave propagation in the two-dimensional photonic crystal deepens the understanding of propagation mechanisms and serves as basis of novel nanodevices.

1. Electromagnetic Wave Propagation in Two-dimensional Photonic Crystal

At ISSSR 2008 it was illustrated that the addition / removal of resonant molecules could alter the propagation in photonic crystals, particularly at the so-called cut-off. Since then we have been investigating the suitability of DNA to serve as the backbone of such a lattice in two regions of the EM spectrum – the Thz and the visible to near UV regimes.

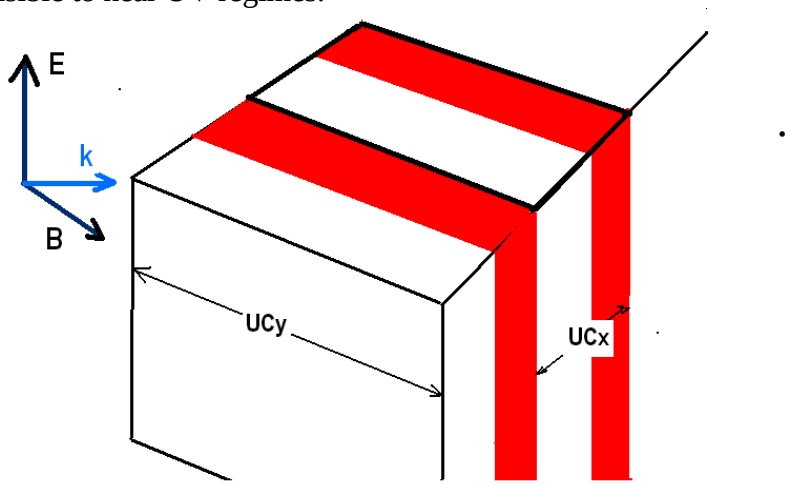

Fig. 1 Scheme of the unit cell

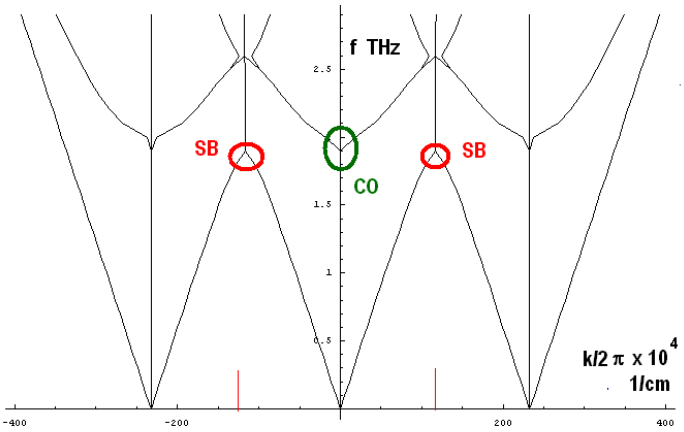

Fig. 2: Frequency vs. K

Fig. 2 shows the frequency behavior in the first Brillouin zone. We are concerned about the change of cut off frequency.

a. Effects of Gold in visible region

Gold is used in order to see the effects of metal on the propagation characteristics. The optical response of Gold can be described as

$$\frac{\varepsilon_{au}}{\varepsilon_0} = 1 - \frac{\omega_p^2}{-i\gamma\omega + \omega^2}$$

Where[1] $\omega_p = 13.8 \times 10^{15}, \gamma = 1.07 \times 10^{14}$.

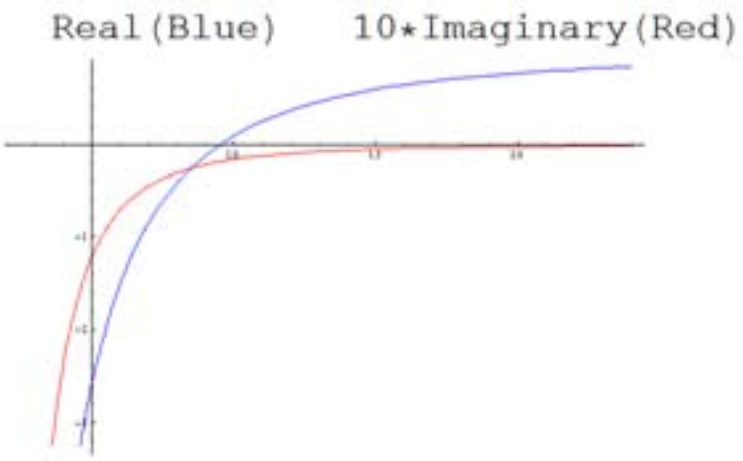

Fig. 3: Metallic response _/ _0

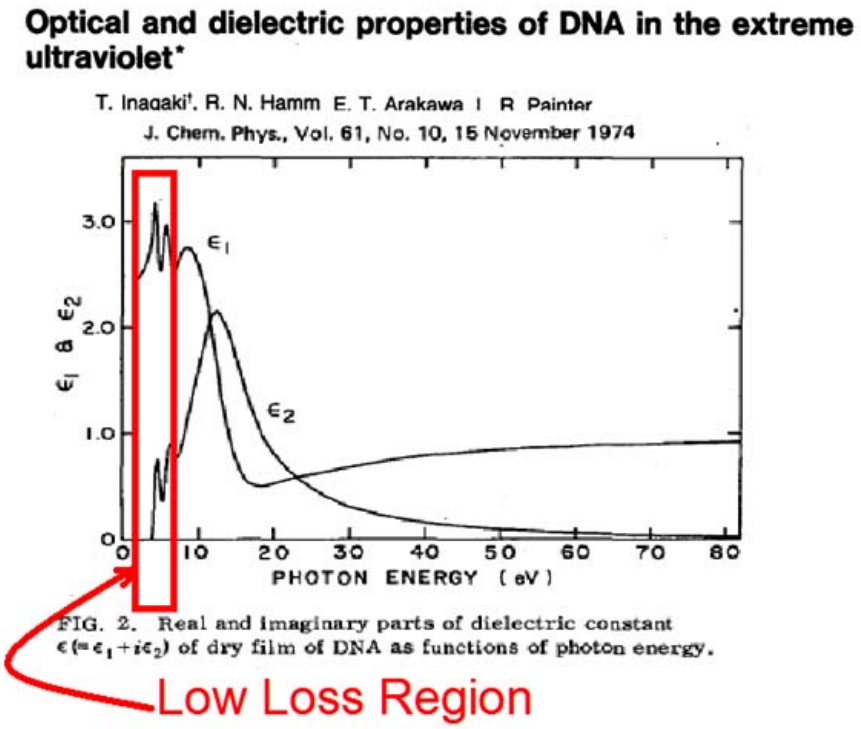

Fig. 4: Optical and dielectric properties of DNA in the extreme ultraviolet

Fig. 5 shows the combined effects of DNA and gold rod, and Fig. 6 illustrates the influences of DNA and gold cube.

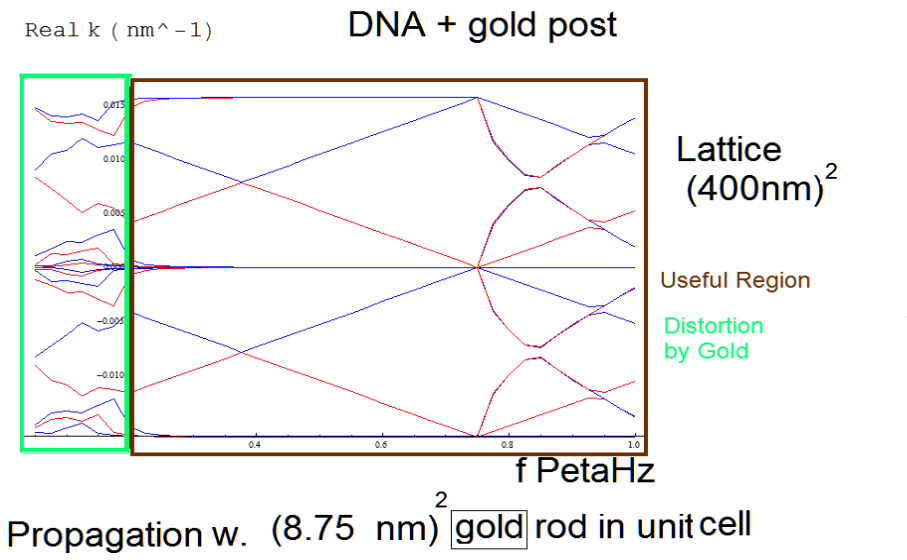

Fig. 5: Real part of wavenumber.

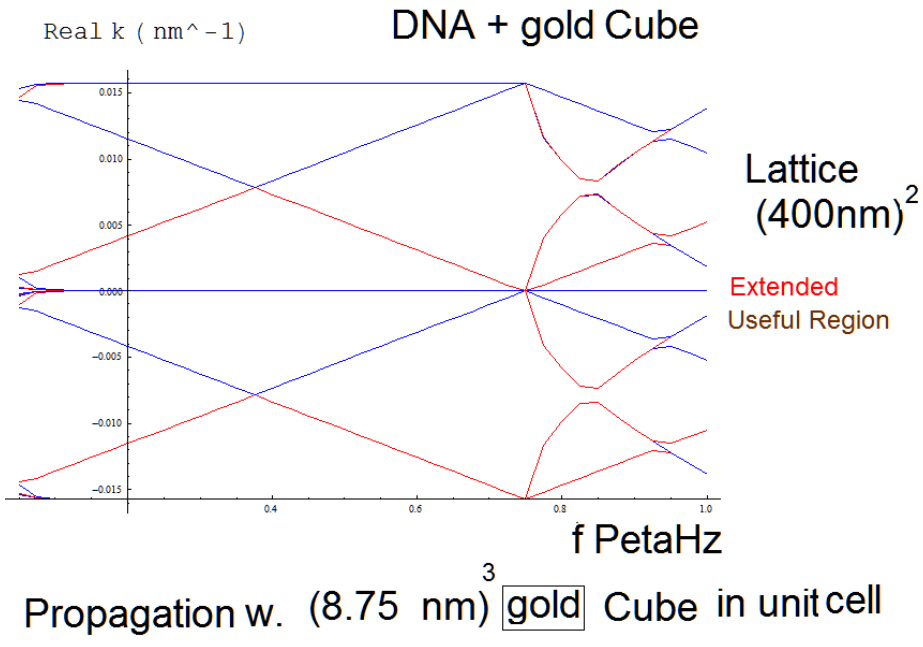

Fig. 6: Real part of wavenumber.

b. Teraherz Propagation

At near-infrared or visible wavelengths, however, it is difficult to manufacture PC structures; the richness of teraherz region in the spectroscopy of small and large molecules in gas and liquid phase together with the ease of fabrication for applications in this wavelength range make PCs attractive for biological and chemical sensing. Relatively large size of lattice – tens of microns -- should permit easy flow of molecules throughout photonic crystal.

Teraherz propagation in the unit cell of DNA lattice[2] has been treated. Change in propagation characteristics can serve as basis for a sensor of a specific gas.

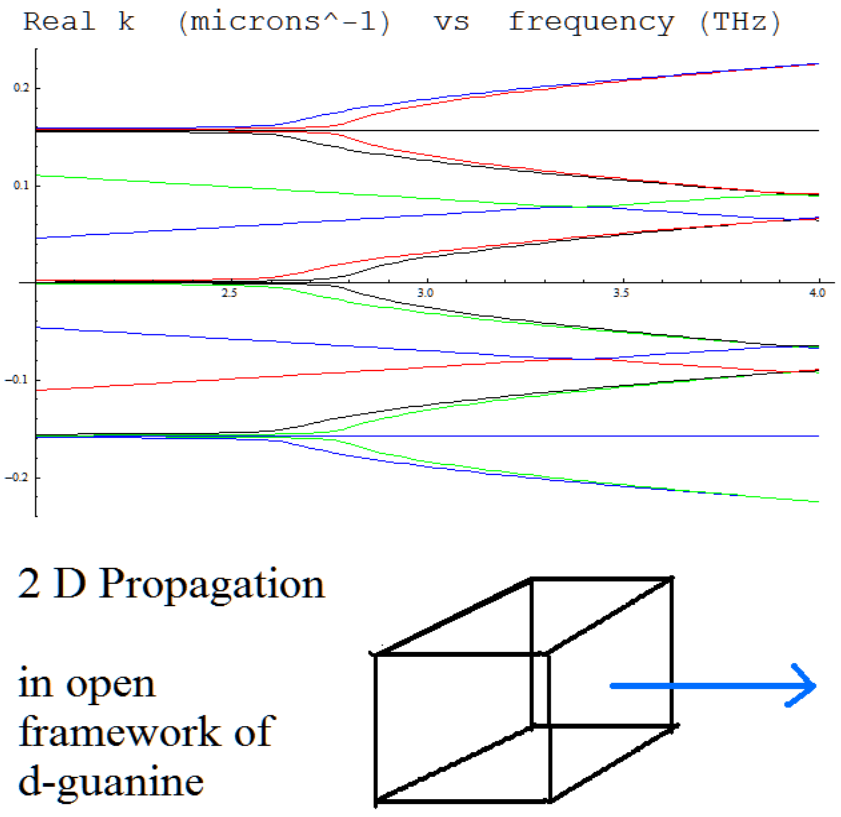

Fig. 7: Real part of wavenumber for frequency in Teraherz region.

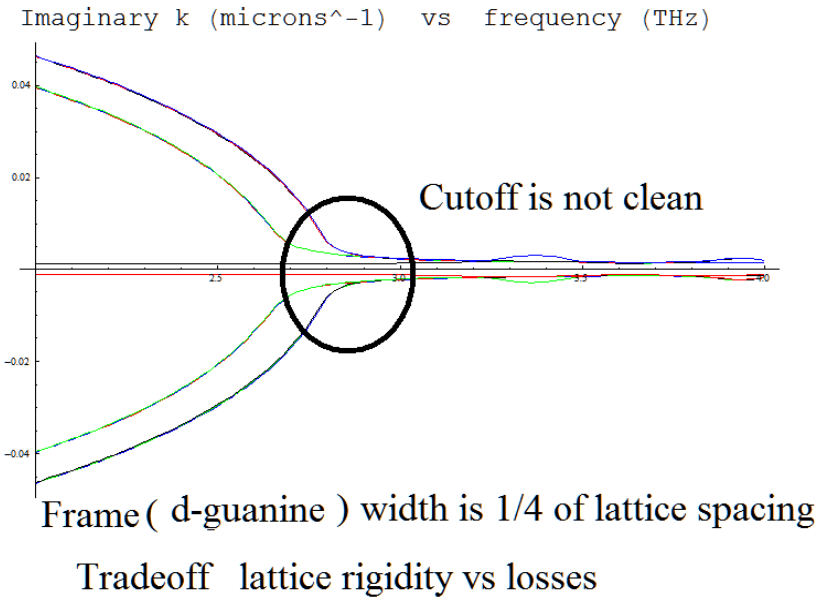

Fig. 8: Imaginary part of wavenumber.

c. Effects of DNA frame

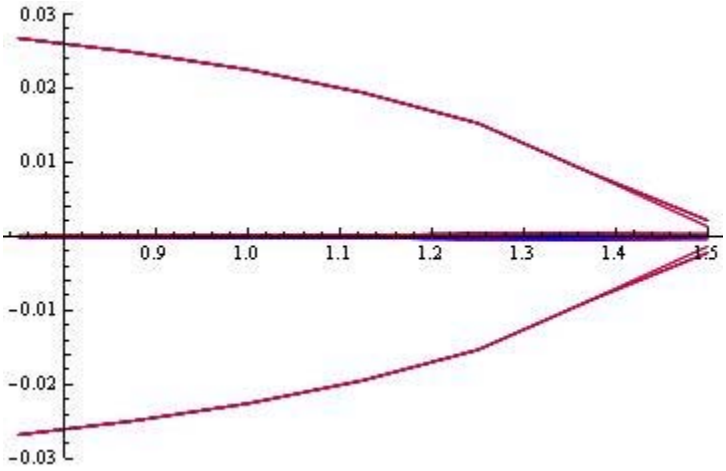

Fig. 9: Imaginary part of wavenumber for thinner DNA frame. No molecule is embedded.

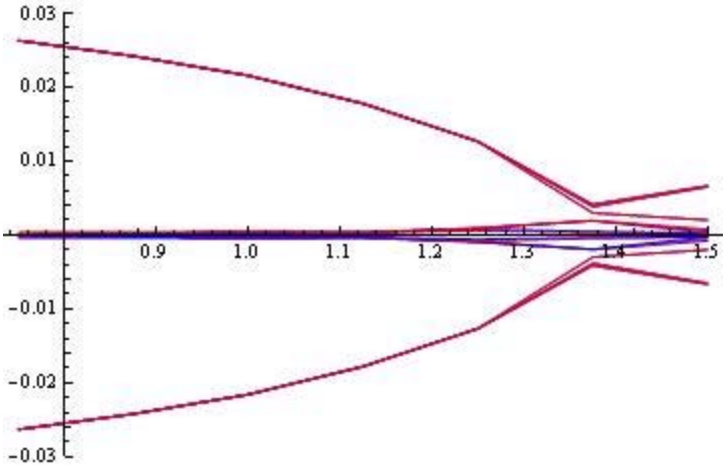

Fig. 10: Imaginary part of wavenumber for thicker DNA frame. No molecule is embedded.

From Figs 9 and 10 it can be seen that DNA contributes to the loss at lower frequenies.

2. Reduction Method

Considerable progress was made in speeding up both the TE and TM codes written in Mathematica by means of compilation. It seems that we can now use Mathematica, with its conveniences, for detailed calculations, even using laptop computers.

A new version of the perturbation scheme has been developed and implemented in (compiled) Mathematica. The basic approximation made is that one can find the propagation characteristics in the first Brillouin zone by considering only those modes which, if uncoupled, would lie in the first two Brillouin zones. A simple and efficient method, which we call the Reduction Method, collapses the mode space appropriately, leading to an eigenvalue equation for the wavenumbers of significantly smaller dimensionality.

The number of modes taken into account is controlled by a single parameter. This permits a simple method of checking the accuracy of the approximation; one need only increase the number of zones included and compare the results.

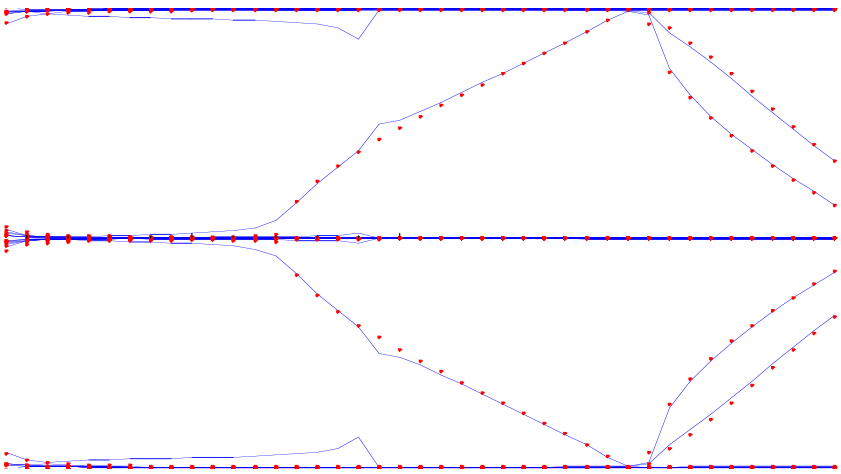

Fig. 11: Real Part of Wave-number (reciprocal nm). Red Dots –Full 81 by 81 matrix; Blue lines 29 by 29 reduced matrix.

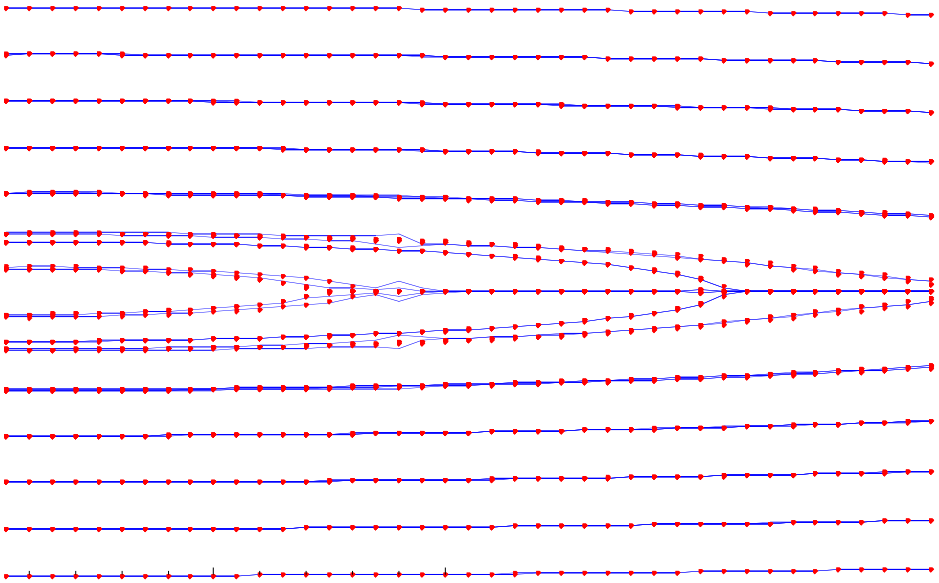

Fig. 12: Imaginary Part of Wave-number (reciprocal nm). Red Dots –Full 81 by 81 matrix; Blue lines 29 by 29 reduced matrix.

3. Summary

The propagation characteristics of DNA in the Thz and visible has been investigated. The results are encouraging.

The effects of metal (gold) placed in each unit cell has been calculated.

Algorithmic advances—perturbation theory and simpler formulation have been made.

Statement of the Problem Studied

We have explored both experimentally and theoretically the issues involved in the preparation of photonic band gap materials using DNA scaffolding for their organization. Experimental approaches entailed learning how to organize materials other than DNA in 2D and in 3D. These included metallic nanoparticles, dyes, DNAzymes and DNA-based nanomechanical devices. A lot of effort was devoted to increasing the sizes of the separations between repeat units in 2D. Small arrays of 100 nm separations were obtained. Macroscopic arrays of 7-14 nanometer separations were also obtained. Theoretical approaches included [1] 2D photonic crystal propagation codes incorporating conductive losses and frequency-dependent materials, and [2] photonic biosensors.

Summary of Most Important Results

Experimental: We have established a number of features of the control of the structure of matter using DNA that have not been described previously. These include the organization of nanoparticles in 2D, the organization of nanomechanical devices in 2D, the organization of DNAzymes in 2D, the longer-distance organization of Rothemund tiles in 1D and 2D and the macroscopic 3D organization of DNA and pendent dyes. All of these advances will serve to build deliberate photonic band gap materials.

Theoretical: [1] The presence of molecules possessing a resonant frequency in the neighborhood of a cutoff region of the photonic crystal can significantly modify the k-characteristics of the lattice from those in the absence of the molecules. In particular, the magnitude of the reflection of waves in the frequency range below cutoff can be lowered because of the raising of the index of refraction by the molecules. This decrease in the attenuation takes place despite the added absorption due to the molecules. To illustrate this effect a computer simulation was carried out in which the dimensions of the unit cell were Lx=43 micros and Ly=110 microns. In each cell half was filled with material for which ε_1=1.33 and the other half with either the molecules described below or with air. The split in properties took place halfway across the unit cell in the x direction, which was the direction of propagation. [2] (a) The propagation characteristics of DNA in the Thz and visible has been investigated. The results are encouraging. (b) The effects of metal (gold) placed in each unit cell has been calculated. (c) Algorithmic advances—perturbation theory and simpler formulation have been made.

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